

# REPORT DOCUMENTATION PAGE

AFRL-SR-BL-TR-00-

JUL 2000

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1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE 00/7/1		3. REPORT TYPE AND DATES COVERED Progress 00/2/15-00/7/1	
4. TITLE AND SUBTITLE (U) PDF Modelling of Turbulent Combustion				5. FUNDING NUMBERS PE-61102F PR-2308 SA-BS, G-F49620-97-1-0126	
6. AUTHOR(S) S.B. Pope					
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Cornell University Ithaca, NY 14853				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/NA 110 Duncan Ave, Suite B115 Bolling AFB Washington, DC 20332-0001				10. SPONSORING / MONITORING AGENCY REPORT NUMBER	
11. SUPPLEMENTARY NOTES					
12a. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release; distribution is unlimited					12b. DISTRIBUTION CODE
13. ABSTRACT (Maximum 200 Words)  Significant progress was made in the application of PDF-based turbulent combustion models to the Sandia pilot-jet nonpremixed flames. These PDF calculations were described in two recent papers (Xu & Pope 2000 and Tang, Xu & Pope 2000) and they are summarized in this report. The first of these works showed that the PDF method is capable of describing, quantitatively, the phenomena of local extinction and reignition (as functions of jet velocity and axial distance) that are observed in these flames. The second paper extended the methodology to include radiative heat loss, and the calculation of NO <sub>x</sub> .					
14. SUBJECT TERMS Turbulent Combustion				15. NUMBER OF PAGES 7	
				16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT Unclassified	20. LIMITATION OF ABSTRACT UL		

DMC QUALITY INSPECTED 4

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NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)  
Prescribed by ANSI Std. Z39-18  
298-102

# PDF MODELLING OF TURBULENT COMBUSTION

AROSR Grant F-49620-00-1-0171

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## SUMMARY

Significant progress was made in the application of PDF-based turbulent combustion models to the Sandia pilot-jet nonpremixed flames. These PDF calculations were described in two recent papers (Xu & Pope 2000 and Tang, Xu & Pope 2000) and they are summarized in this report. The first of these works showed that the PDF method is capable of describing, quantitatively, the phenomena of local extinction and reignition (as functions of jet velocity and axial distance) that are observed in these flames. The second paper extended the methodology to include radiative heat loss, and the calculation of  $NO_x$ .

## PDF MODEL

The model is based on the transport equation for the joint probability density function of velocity, turbulence frequency and thermochemical composition. For the combustion of methane considered, the chemical kinetics are represented by the augmented reduced mechanism of Sung, Law & Chen (1998). Without  $NO_x$  chemistry (ARM1) there are 16 species; with  $NO_x$  there are 19. For computational tractability, the effects of reaction are implemented by the in situ adaptive tabulation (ISAT) algorithm (Pope 1997).

## LOCAL EXTINCTION

The piloted jet nonpremixed flames measured by Barlow & Frank (1998) consist of a central jet of methane, a substantial annular pilot, and coflowing air. In the three flames considered, *D*, *E* and *F*, the jet velocities are  $U_J = 50, 74$  and  $99$  m/s, respectively. The amount of local extinction increases with the jet velocity.

Figure 1 shows scatter plots of the  $CO_2$  mass fraction against mixture fraction for Flame *F* at 30 jet radii downstream. In the measurements (left-hand figure), each point represents a laser shot; in the calculations (right-hand figure), each point represents a particle from the particle/mesh method used to solve the PDF equation. The upper curve is the composition of a mildly strained laminar flame. The fact that the bulk of the points lie beneath this line is an indication of local extinction. The lower curve is the conditional mean from the data. Good agreement between the calculations and the measurements may be observed.

Xu & Pope (2000) define a "burning index" (BI) as a measure of (the lack of) local extinction. To explain the definition of the burning index we again refer to Fig. 1.

The vertical dashed line shows a mixture fraction range around strichiometric (defined by Barlow & Frank 1998). The lower solid circle is the mean of the data points that lie in this range; whereas the upper solid circle is the value from the laminar flame. The burning index is defined as the ratio of these two values. Consequently, a burning index of 1 corresponds (roughly) to complete combustion, and 0 corresponds to complete extinction.

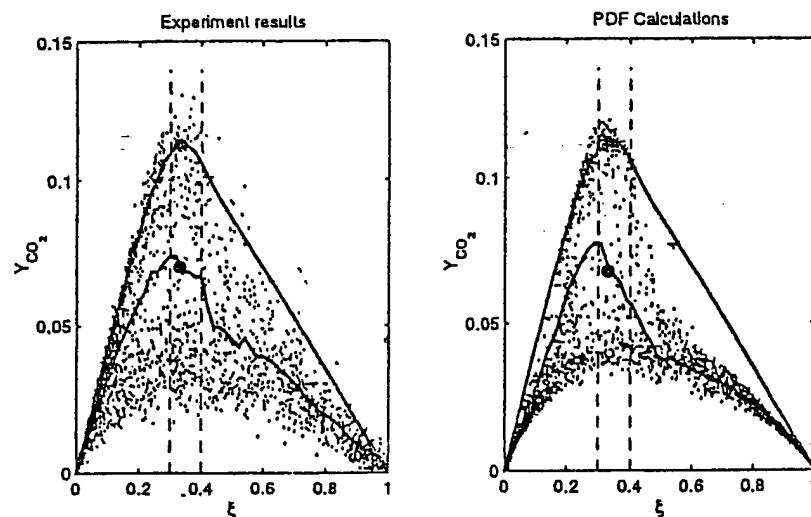


Figure 1: Scatter plots of  $CO_2$  mass fraction against mixture fraction for flame  $F$  at an axial distance of 15 jet diameters. Left-hand plot, experimental data of Barlow & Frank (1998); right-hand plot, PDF calculations of Xu & Pope (2000).

Figure 2 compares the measured and calculated burning indexes of different species (and temperature) for all three flames as functions of axial distance. As may be seen, with few exceptions, the PDF calculations accurately describe the dependence of BI on both the jet velocity and on the axial distance. These results demonstrate a significant advance in our abilities to calculate substantial finite-rate chemistry-turbulence interactions.

## MAJOR AND MINOR SPECIES

For flame  $D$ , Fig. 3 shows calculated radial profiles of the mean and r.m.s. of the  $NO$  mass fraction compared to the experimental data. Good agreement may be observed for both quantities, and the downstream evolution is well represented. It may be seen that radiative heat loss does not have a significant impact on  $NO$  (in this flame).

Figure 4 shows the conditional mean (conditioned on mixture fraction  $\xi$ ) of various quantities. These conditional means provide a good indication of the accuracy of the chemistry calculations. As may be seen, the agreement between the calculations and the experiments is uniformly satisfactory. The trends of  $NO$  with jet velocity and downstream distance are accurately represented; and the accuracy of the  $CO$  calculations shows that ARM remedies previously observed discrepancies.

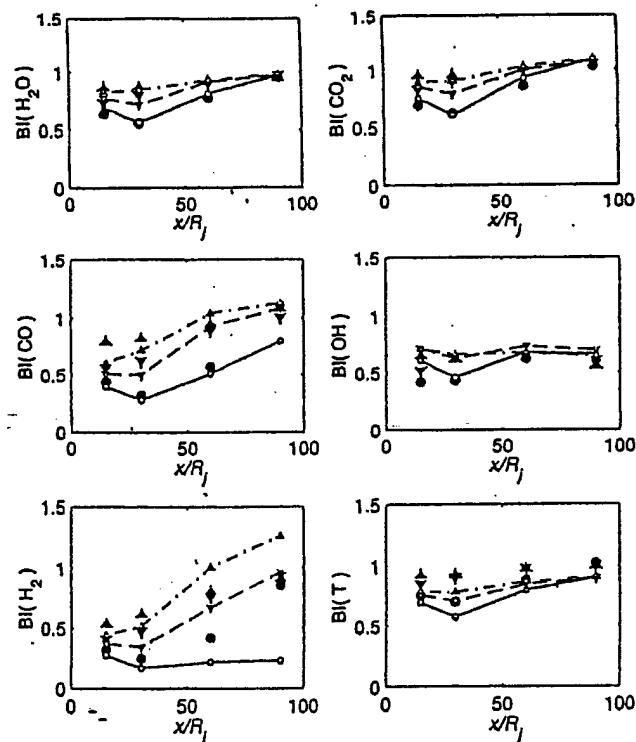


Figure 2: Burning indexes for flames *D*, *E* and *F*. Filled symbol: experiments; lines with empty symbols, PDF calculations. Circle and solid line, flame *F*; down-triangle and dashed line, flame *E*; up-triangle and dashed-dotted line, flame *D*. (From Xu & Pope 2000.)

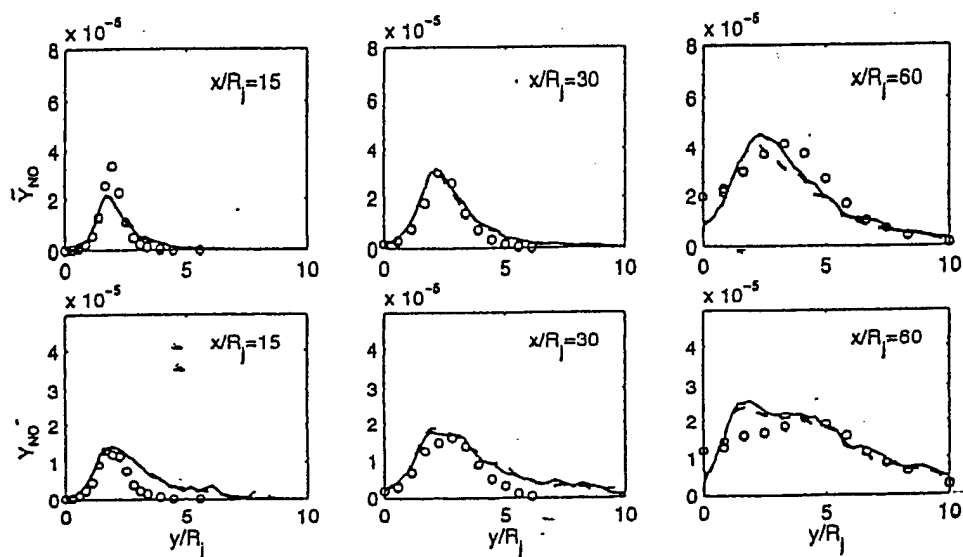


Figure 3: Radial profiles of the mean (upper plots) and r.m.s. (lower plots) of  $NO$  mass fraction in flame *D*. Symbols, experimental data (Barlow & Frank 1998); solid and dashed lines, PDF calculations without and with radiative heat loss. (From Tang, Xu & Pope 2000.)

## REFERENCES

1. Barlow R.S. and Frank J.H. "Effects of turbulence on species mass fraction in methane/air jet flames," In *Twenty-seventh Symp. (Int'l) on Combust.*, page 1087, Pittsburgh, 1998. The Combustion Institute.
2. Pope S.B. (1997) "Computationally Efficient Implementation of Combustion Chemistry using In Situ Adaptive Tabulation," *Combustion Theory and Modelling*, 1, 41-63.
3. Sung, C. J., Law C. K., and Chen J.-Y. (1998). "An augmented reduced mechanism for methane oxidation with comprehensive global parametric validation." In *Twenty-seventh Symp. (Int'l) on Combust.*, Pittsburgh, pp. 295-304. The Combustion Institute.
4. Tang Q., Xu J. and Pope S.B. (2000) "PDF calculations of local extinction and NO production in piloted-jet turbulent methane/air flames", *Twenty-Eighth Symp. (Int'l) on Combust.* (to be published).
5. Xu J. and Pope S.B. (2000) "PDF calculations of turbulent nonpremixed flames with local extinction," *Combust. Flame* (to be published).

## PERSONNEL SUPPORTED

Prof. S.B. Pope, PI  
S. Joseph, graduate student  
Q. Tang, graduate student

## DEGREES GRANTED

S. Joseph, M.S.

## PUBLICATIONS

The following papers were written during the reporting period.

1. Q. Tang, J. Xu and S.B. Pope (2000) "PDF calculations of local extinction and NO production in piloted-jet turbulent methane/air flames," *Twenty-Eighth Symp. (Int'l) on Combust.* (to be published).
2. J. Xu and S.B. Pope (2000) "PDF calculations of turbulent nonpremixed flames with local extinction," *Combust. Flame* (to be published).

## PRESENTATIONS

June 5, 2000—University of California, Santa Barbara, Institute of Theoretical Physics.

June 13, 2000—AFOSR/ARO Contractors' Meeting, Workshop presentation, Santa Fe, NM.

July 27, 2000—Fifth International Workshop on Nonpremixed Turbulent Combustion, Delft, Netherlands.

July 31, 2000—International Combustion Symposium, presentation.

## OTHER INTERACTIONS

During the reporting period the PI has visited:

Rolls Royce Corporation, Indianapolis, IN

Rocketdyne, Canoga Park, CA

Los Alamos National Lab, NM

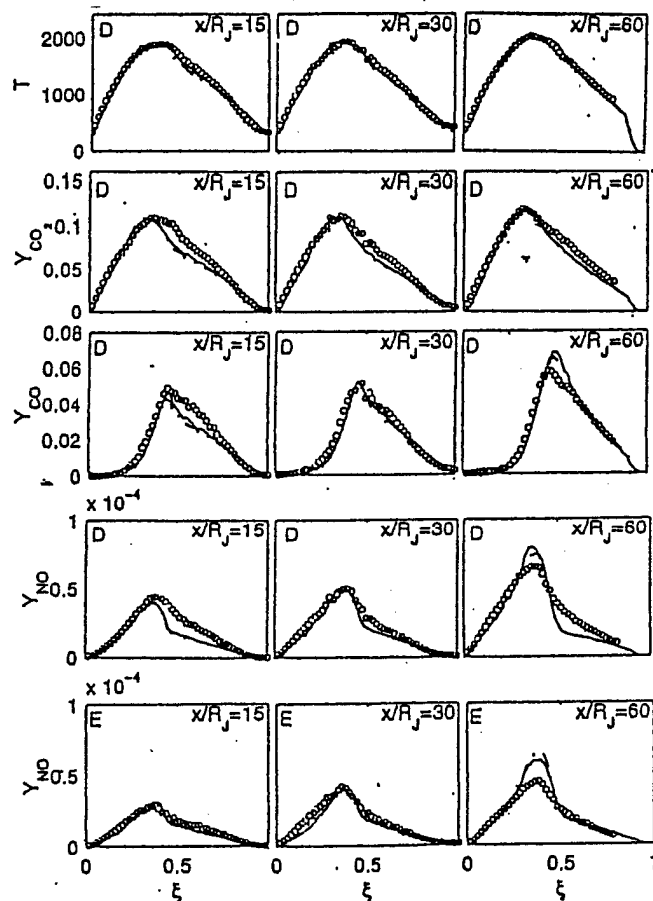


Figure 4: Conditional means in flames  $D$  and  $F$ . Lines and symbols as in Fig. 3.

Principal Investigator Annual Data Collection (PIADC) Survey Form

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PI DATA

Name (Last, First, MI) Pope, Stephen B.  
Institution Cornell University  
Contract/Grant No F4962-00-1-0171

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Project/Subarea \_\_\_\_\_/\_\_\_\_\_

NX \_\_\_\_\_

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NUMBER OF CONTRACT/GRANT CO-INVESTIGATORS

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PUBLICATIONS RELATED TO AFOREMENTIONED CONTRACT/GRANT

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Do Not Include: Honors and awards unrelated to the scientific field covered by the contract/grant.

Honor/Award Fellow, American Physical Society Year Received: 1991

Honor/Award Recipient(s) S.B. Pope

Awarding Organization American Physical Society

Associate Fellow 1984  
S.B. Pope  
AIAA

Overseas Fellow 1989  
S.B. Pope  
Churchill College, Cambridge